

Isoscalar and isovector pairing in a formalism of quartets

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Abstract

Isoscalar ($T = 0, J = 1$) and isovector ($T = 1, J = 0$) pairing correlations in the ground state of self-conjugate nuclei are treated in terms of alpha-like quartets built by two protons and two neutrons coupled to total isospin $T = 0$ and total angular momentum $J = 0$. Quartets are constructed dynamically via an iterative variational procedure and the ground state is represented as a product of such quartets. It is shown that the quartet formalism describes accurately the ground state energies of realistic isovector plus isoscalar pairing Hamiltonians in nuclei with valence particles outside the ^{16}O , ^{40}Ca and ^{100}Sn cores. Within the quartet formalism we analyse the competition between isovector and isoscalar pairing correlations and find that for nuclei with the valence nucleons above the cores ^{40}Ca and ^{100}Sn the isovector correlations account for the largest fraction of the total pairing correlations. This is not the case for sd -shell nuclei for which isoscalar correlations prevail. Contrary to many mean-field studies, isovector and isoscalar pairing correlations mix significantly in the quartet approach.

Keywords: self-conjugate nuclei, isovector-isoscalar pairing, quartet formalism

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1. Introduction

One of the most debated and yet open issues in nuclear physics is whether or not the deuteron-like proton-neutron pairs of isospin $T = 0$ and angular momentum $J = 1$ behave coherently in the form of a condensate, analogous in structure to the condensates of like-particle pairs. For about 50 years the isoscalar proton-neutron pairing and its competition with the isovector ($T = 1, J = 0$) pairing have been commonly studied in the framework of the Hartree-Fock-Bogoliubov (HFB) theory. Most of its developments, starting from the pioneering works [1, 2, 3, 4] have been reviewed by Goodman [5, 6] (for a recent study, see [7]). However, as clearly evidenced in applications within exactly solvable models of $T = 1$ and $T = 0$ pairing [8, 9, 10, 11], this theory suffers important limitations due to its inherent violations of the particle number and of the isospin. Such violations are, of course, absent in the Shell Model (SM) and various attempts have been made to employ this approach to elucidate the competition between the isoscalar and isovector pairing correlations [12, 13]. However, it is still unclear how one could identify in the complicated SM wave function the existence of the collective pairs and their possible coherence in the form of a pair condensate.

In the present study we propose a new approach for treating the isoscalar and isovector pairing interaction in $N = Z$ nuclei which is based not on pairs, as in the case of the HFB theory, but on alpha-like quartets. This approach presents the advantage of conserving exactly the particle number and the isospin and, at the same time, it is simple enough for understanding the role played by the isoscalar and isovector pairing correlations.

The idea of using quartets for describing proton-neutron pairing in nuclei is rather old [14] but it has been mostly employed for treating the isovector interaction [15, 16, 17, 18, 19]. A consistent quartet formalism for treating the isovector pairing, which conserves the particle number, the isospin and takes into account exactly the Pauli blocking, has been proposed in Refs. [20, 21]. In this model the ground state of $N = Z$ nuclei is approximated by a condensate of

alpha-type quartets formed by two isovector pairs coupled to $T = 0$. Recently this model has been generalized by allowing the isovector quartets to be different from one another [22]. In the present letter we extend the quartet model to the treatment of both the isovector and the isoscalar pairing interactions in nuclei with an equal number of protons and neutrons outside a self-conjugate core.

The manuscript is structured as follows. In Section 2, the ground state of the isovector plus isoscalar Hamiltonian for $N = Z$ systems is formulated in the formalism of quartets. In Section 3, the quartet formalism is applied to nuclei with valence particles outside the ^{16}O , ^{40}Ca and ^{100}Sn . Finally, in Section 4, we give the conclusions.

2. The quartet formalism

The isovector plus isoscalar pairing Hamiltonian in a spherically symmetric mean field has the form

$$H = \sum_i \epsilon_i N_i + \sum_{i,j} V_{J=0}^{T=1}(i,j) \sum_{T_z} P_{i,T_z}^+ P_{j,T_z} + \sum_{i \leq j, k \leq l} V_{J=1}^{T=0}(ij,kl) \sum_{J_z} D_{ij,J_z}^+ D_{kl,J_z}. \quad (1)$$

In the first term, ϵ_i and N_i are, respectively, the energy and the particle number operator relative to the single-particle state i . The symbol i is a short cut notation for $\{n_i, l_i, j_i, \tau_i\}$, with $\{n_i, l_i, j_i\}$ being the standard orbital quantum numbers and τ_i denoting the isospin projection. The Coulomb interaction between the protons is not taken into account so that the single-particle energies of protons and neutrons are assumed to be equal. The second term in Eq. (1) is the isovector pairing interaction. This is formulated in terms of the non-collective pair operators

$$P_{i,T_z}^+ = \frac{1}{\sqrt{2}} [a_i^+ a_i^+]_{T_z}^{T=1, J=0} \quad (2)$$

where T_z denotes the three projections of the isospin $T = 1$ corresponding to neutron-neutron ($T_z = 1$), proton-proton ($T_z = -1$) and proton-neutron ($T_z = 0$) pairs. The isoscalar pairing interaction, the third term in Eq. (1), is

written in terms of the pair operators

$$D_{ij,J_z}^+ = \frac{1}{\sqrt{1 + \delta_{ij}}} [a_i^+ a_j^+]_{J_z}^{J=1, T=0} \quad (3)$$

where J_z denotes the three projections of the angular momentum $J = 1$.

It is worth mentioning that the Hamiltonian (1) is exactly solvable only for $V_{J=0}^{T=1}(i, j) = V_{J=1}^{T=0}(ij, kl) = g$, where g is a state-independent pairing strength, and in the absence of the spin-orbit interaction. In this case, the isovector and isoscalar correlations play a similar role and contribute to the ground state energy to an equal amount [11].

In this work we investigate to which extent the ground state of the Hamiltonian (1) for an even-even self-conjugate nucleus can be represented in terms collective alpha-like quartets having total angular momentum $J = 0$ and total isospin $T = 0$. One can form two types of quartets: isovector quartets, resulting from the coupling of two isovector pairs (2),

$$Q_\nu^{+(iv)} = \sum_{i,j} x_{ij}^{(\nu)} [P_i^+ P_j^+]^{T=0} \quad (4)$$

and isoscalar quartets, formed instead by two isoscalar pairs (3)

$$Q_\nu^{+(is)} = \sum_{ij,kl} y_{ij,kl}^{(\nu)} [D_{ij}^+ D_{kl}^+]^{J=0}. \quad (5)$$

By summing up these quartets one constructs the generalized quartets

$$Q_\nu^+ = Q_\nu^{+(iv)} + Q_\nu^{+(is)}. \quad (6)$$

We approximate the ground state of the Hamiltonian (1) for an even-even $N = Z$ nucleus as a product of such quartets, namely

$$|\Psi_{gs}\rangle \equiv |QM\rangle = \prod_{\nu=1}^{N_Q} Q_\nu^\dagger |0\rangle \quad (7)$$

where $|0\rangle$ denotes a self-conjugate core of nucleons not affected by the pairing interaction. Since each quartet has $T = 0$ and $J = 0$, these also represent the quantum numbers of the ground state (7). Dealing with $T = 0$ and $J = 0$ quartets only has the great advantage of not requiring any angular momentum

coupling, but also is simpler to apply than that proposed in Ref. [23] which instead employed general quartets with $J \neq 0$, $T \neq 0$.

The QM state depends on the mixing amplitudes $x_{ii'}^{(\nu)}$ and $y_{ii',jj'}^{(\nu)}$ which define the collective isovector and isoscalar quartets. In order to find them we employ a generalization of the iterative variational procedure used in the case of the isovector pairing [22] (for details, see also [24, 25]). The procedure consists of a sequence of diagonalizations of the Hamiltonian (1) in spaces whose size N_q is given by the total number of non-collective isovector ($[P_i^+ P_j^+]^{T=0}$) and isoscalar ($[D_{ij}^+ D_{kl}^+]^{J=0}$) quartets which can be formed in the chosen model space of single-particle states. For simplicity, we denote all these non-collective quartets as q_μ^+ ($\mu = 1, 2, \dots, N_q$) and write the collective quartet (6) generically as $Q_\nu^+ = \sum_\mu c_\mu^{(\nu)} q_\mu^+$. In order to describe a system with N_Q quartets, we proceed step-by-step starting from the case of one quartet. For $N_Q = 1$, the Hamiltonian (1) is diagonalized in the space F_1 spanned by all possible non-collective quartets, i.e. $F_1 = \{q_\mu^+ | 0\rangle\}$. The lowest state in energy which results from this diagonalization represents the exact ground state for the system with two neutrons and two protons and it has the form $|\Psi_1\rangle = Q_1^+ | 0\rangle$. For the system with $N_Q = 2$ quartets, as a first approximation of the ground state, we assume the lowest state in energy resulting from the diagonalization of H in the space $F_2^{(1)} = \{q_\mu Q_1^+ | 0\rangle\}$, where Q_1^+ is the quartet previously determined. This state has therefore the form

$$|\Psi_2^{(1)}\rangle = Q_2^+ Q_1^+ | 0\rangle \equiv Q_2^+ |\Psi_1\rangle. \quad (8)$$

From this point on, a series of diagonalizations starts whose purpose is that of finding the quartets which guarantee the lowest possible energy of the state (8). Each diagonalization is meant to update one quartet while leaving the other unchanged. In the second step, for instance, one proceeds by diagonalizing H in the space $F_2^{(2)} = \{q_\mu Q_2^+ | 0\rangle\}$. This diagonalization generates the second order approximation for the ground state

$$|\Psi_2^{(2)}\rangle = Q_1^{+(new)} Q_2^+ | 0\rangle. \quad (9)$$

This state is expected to be lower (or, at worst, equal) in energy with respect to $|\Psi_2^{(1)}\rangle$ and so each diagonalization, while updating a quartet, drives the two-quartet state toward its minimum in energy. This diagonalization is iterated until the energy converges.

The procedure illustrated in the previous paragraph for the case $N_Q = 2$ can be generalized for any value of N_Q . In general, if Q_ν^\dagger ($\nu = 1, 2, \dots, N_Q - 1$) are the final quartets generated for the system $N_Q - 1$, we start by finding the lowest order approximation of the ground state for the system with N_Q quartets, which results from the diagonalization of H in the space

$$F_{N_Q}^{(1)} = \left\{ q_\mu^+ \prod_{\nu=1}^{N_Q-1} Q_\nu^\dagger |0\rangle \right\} \equiv \left\{ q_\mu^+ |\Psi_{N_Q-1}\rangle \right\} \quad (10)$$

and it has therefore the form

$$|\Psi_{N_Q}^{(1)}\rangle = Q_{N_Q}^+ |\Psi_{N_Q-1}\rangle. \quad (11)$$

This lowest order approximation is improved by an iterative sequence of diagonalizations which updates the quartets one by one and drives this state towards its minimum in energy.

It is worthy noticing that, owing to this continuous updating, the quartets that populate the final state $|\Psi_{N_Q}\rangle$ are different from those defining $|\Psi_{N_Q-1}\rangle$. In this sense, quartets are generated dynamically for every N_Q . This fact makes impossible to establish a simple connection between $|\Psi_{N_Q}\rangle$ and $|\Psi_{N_Q-1}\rangle$. However, as evidenced in Eq. (11), if the iterative procedure is arrested at the lowest order, the ground state at this stage, $|\Psi_{N_Q}^{(1)}\rangle$, simply results from the action of a quartet creation operator on the ground state for $N_Q - 1$. This expression is of particular interest because, provided that $|\Psi_{N_Q}^{(1)}\rangle$ can be proved to be a good approximation of the exact ground state, it would give a clear evidence of the key role played by $T = 0$, $J = 0$ quartets in the ground state of the isovector-isoscalar pairing Hamiltonian.

3. Results

To test the accuracy of the quartet model we have performed calculations for three sets of $N = Z$ nuclei with valence nucleons outside the ^{16}O , ^{40}Ca , and ^{100}Sn cores. The isovector and isoscalar pairing forces of the Hamiltonian (1) have been extracted, respectively, from the $(T = 1, J = 0)$ and $(T = 0, J = 1)$ components of standard shell model interactions. More precisely, for nuclei outside the ^{16}O core we have used the USDB interaction [26], for those outside the ^{40}Ca core the monopole-modified Kuo-Brown interaction KB3G [12] and, for those outside the ^{100}Sn core, the effective G-matrix interaction of Ref. [27]. As single-particle energies we have taken those employed with the previous interactions (e.g., see Ref. [20]).

The results for the pairing correlation energy, defined as the difference between the ground state energies obtained with and without the pairing force, are given in Table 1. In order to check the accuracy of the quartet model, the calculations have been done only for those $N = Z$ nuclei for which the Hamiltonian (1) could be diagonalized exactly. As seen in Table 1, the errors relative to the exact solution are very small, under 1%. This shows that the ansatz (7) for the ground state is a very good approximation for describing the isoscalar-isovector pairing correlations.

In Table 1 we also present the results relative to the lowest order approximation (11). In addition to the correlation energies, we show the overlaps between this approximated ground state and the actual QM ground state, i.e. the state at the end of the iterative process. It can be seen that the relative errors remain confined within 1% even in this case and that these overlaps are very close to 1. Therefore the lowest order approximation too emerges as an excellent approximation of the exact ground state.

Having verified that the QM state (7) is able to describe with very high precision the pairing correlation energies of the isovector plus isoscalar Hamiltonian (1), the quartet formalism can be used to analyse the competition between the isovector and isoscalar components of the pairing interaction. Due to the mixed

Table 1: Ground state correlation energies (in MeV) calculated for the isovector plus isoscalar pairing Hamiltonian (1) with strengths extracted from standard shell model interactions (see text). The results are shown for the exact diagonalization, the QM state (7) and the lowest order approximation (11), denoted by QM(l.o.). The errors relative to the exact results are given in brackets. Overlaps (in absolute values) between the states QM and QM(l.o.) are reported in the last column.

	Exact	QM	QM(l.o.)	$\langle QM QM(l.o.)\rangle$
^{24}Mg	28.694	28.626 (0.24%)	28.592 (0.35%)	0.9993
^{28}Si	35.600	35.396 (0.57%)	35.307 (0.82%)	0.9980
^{32}S	38.965	38.865 (0.25%)	38.668 (0.76%)	0.9942
^{48}Cr	11.649	11.624 (0.21%)	11.614 (0.30%)	0.9996
^{52}Fe	13.887	13.828 (0.43%)	13.804 (0.60%)	0.9994
^{108}Xe	5.505	5.495 (0.18%)	5.490 (0.27%)	0.9995
^{112}Ba	7.059	7.035 (0.34%)	7.025 (0.48%)	0.9987

nature of the quartets, Eq. (6), the QM ground state (7) contains an isovector component

$$|iv\rangle = \prod_{\nu=1}^{N_Q} Q_{\nu}^{\dagger(iv)}|0\rangle, \quad (12)$$

an isoscalar component

$$|is\rangle = \prod_{\nu=1}^{N_Q} Q_{\nu}^{\dagger(is)}|0\rangle \quad (13)$$

and, for $N_Q > 1$, a mixed component with both isovector and isoscalar quartets. As all these components are not orthogonal to each other, it is not trivial to analyse their competition in the ground state. Thus in order to explore the relative importance of the isovector and isoscalar correlations, we have carried out two further QM calculations, one by assuming a ground state formed only by isovector quartets, i.e. of the type (12), and the other with a ground state formed only by isoscalar quartets, i.e. of the type (13). The results of these calculations are presented in Table 2 where we report the ground state correlation energies in the different approximations and the overlaps between the corresponding wave

functions. One can see that, for nuclei with valence nucleons outside the ^{40}Ca and ^{100}Sn cores, the isovector quartet state (12) is able to account for the largest part of the correlation energy induced by the isovector-isoscalar interaction. This fact is also supported by the large overlaps with the QM state (7). However, the isoscalar correlation contribution remains non-negligible because, as seen in Table 1, it reduces the errors in the correlation energies by about one order of magnitude. A different situation is observed instead in the case of *sd*-nuclei where the pairing forces extracted from the USDB shell-model interaction give rise to a prominence of the isoscalar contribution. Still in Table 2 one can notice that the overlap between the isovector-type (12) and isoscalar-type (13) ground states can be rather large. This overlap is a measure of the difficulty in disentangling the isovector and isoscalar contributions. It is worth mentioning that in the present symmetry conserving quartet formalism the isovector and isoscalar pairing correlations always coexist, which is usually not the case in HFB calculations [6, 7].

Previous works (e.g., see Refs. [7, 13]) have evidenced a strong effect of the spin-orbit interaction on the interplay between isovector and isoscalar correlations. We have investigated this effect in the case of *pf*-shell nuclei by repeating the QM calculations in the absence of the single-particle energy splittings induced by the spin-orbit interaction. In particular, we have assumed all single particle energies equal to 2.6 MeV (roughly speaking the centroid of the original single particle energies [12]) and kept unchanged the isovector and isoscalar strengths in the Hamiltonian (1). The new results appear to be reversed with respect to those shown in Table 2, with the isoscalar quartet state (13) accounting for the largest fraction of the correlation energy induced by the isovector-isoscalar interaction (the deviations from the QM values are now confined within 5% while they become larger than 20% for the isovector state (12)). Also the overlaps between the corresponding states appear to be reversed with $\langle QM|is\rangle$ being now close to 0.9. Our analysis within the quartet formalism therefore confirms that isoscalar correlations are strongly hindered by the spin-orbit interaction in these nuclei.

Table 2: Correlation energies (in MeV) calculated with the isovector quartet state (12) and the isoscalar quartet state (13). In the first column we give, as a reference, the results corresponding to the full QM state (7). The errors relative to the QM results are shown in brackets. In the three columns on the right we report the overlaps (in absolute values) between the quartet states just mentioned.

	QM	iv	is	$\langle QM iv\rangle$	$\langle QM is\rangle$	$\langle iv is\rangle$
^{20}Ne	15.985	14.402 (9.9%)	15.130 (5.4%)	0.884	0.953	0.843
^{24}Mg	28.626	23.269 (18.7%)	26.925 (5.9%)	0.650	0.911	0.336
^{28}Si	35.396	28.897 (18.4%)	33.376 (5.7%)	0.590	0.911	0.343
^{32}S	38.865	33.959 (12.6%)	37.884 (2.5%)	0.638	0.973	0.595
^{44}Ti	7.019	6.274 (10.6%)	4.917 (30.0%)	0.901	0.678	0.303
^{48}Cr	11.624	10.589 (8.9%)	7.384 (36.5%)	0.906	0.497	0.221
^{52}Fe	13.828	12.814 (7.3%)	9.980 (27.8%)	0.927	0.753	0.746
^{104}Te	3.147	3.041 (3.4%)	1.549 (50.8%)	0.978	0.489	0.314
^{108}Xe	5.495	5.240 (4.6%)	2.627 (52.2%)	0.958	0.354	0.234
^{112}Ba	7.035	6.614 (6.0%)	4.466 (36.5%)	0.939	0.375	0.376

4. Conclusions

In this work we have described the ground state of the isovector plus isoscalar pairing Hamiltonian in even-even $N = Z$ nuclei in a formalism of alpha-like quartets. Quartets are built by two neutrons and two protons coupled to total isospin $T = 0$ and total angular momentum $J = 0$. The ground state is represented as a product of quartets and a procedure to construct them has been described. The formalism does not violate any symmetry of the Hamiltonian. We have carried out a number of numerical tests for systems with valence nucleons outside the ^{16}O , ^{40}Ca and ^{100}Sn cores and with pairing interactions extracted from realistic shell model Hamiltonians. We have verified that ground state correlation energies are reproduced with high accuracy in the quartet formalism. For the same

systems we have shown that, to a very good extent, the $T = 0$, $J = 0$ quartets link the pairing ground states of adjacent even-even $N = Z$ nuclei. Therefore the role played by these quartets in even-even self-conjugate nuclei appears analogous to that of Cooper pairs in the ground state of a like-particle pairing Hamiltonian. We have also analyzed the competition between the isovector and isoscalar pairing within the quartet formalism. Isovector pairing correlations have been found dominant in the ground states of pf -shell nuclei and of nuclei outside the ^{100}Sn core while, in sd -shell nuclei, the isoscalar pairing correlations have been found to prevail. A strong mixing between isovector and isoscalar pairing correlations has been observed in most of the cases. Finally, we have analyzed the effect of the spin-orbit interaction on the interplay between isovector and isoscalar correlations in pf -shell nuclei. Consistently with previous works, we have found that this interplay is strongly affected by this interaction and that, in his absence, isoscalar correlations become the dominant ones.

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